

# Complexity of Single-Swap Heuristics for Metric Facility Location and Related Problems\*

Sascha Brauer

sascha.brauer@uni-paderborn.de

Department of Computer Science  
Paderborn University  
33098 Paderborn, Germany

Metric facility location and  $K$ -means are well-known problems of combinatorial optimization. Both admit a fairly simple heuristic called *single-swap*, which adds, drops or swaps open facilities until it reaches a local optimum. For both problems, it is known that this algorithm produces a solution that is at most a constant factor worse than the respective global optimum. In this paper, we show that single-swap applied to the weighted metric uncapacitated facility location and weighted discrete  $K$ -means problem is tightly PLS-complete and hence has exponential worst-case running time.

## 1 Introduction

Facility location is an important optimization problem in operations research and computational geometry. Generally speaking, the goal is to choose a set of locations, called facilities, minimizing the cost of serving a given set of clients. The service cost of a client is usually measured in some form of distance from the client to its nearest open facility. To prevent the trivial solution of opening a facility at each possible location, we usually introduce some sort of opening cost penalizing large sets of open facilities. This general framework comprises a plethora of problems using different functions to measure distance and combinations of opening and service cost. In this paper, we discuss two popular problems closely related to facility location: METRIC UNCAPACITATED FACILITY LOCATION (MUFL) and DISCRETE  $K$ -MEANS (DKM).

### 1.1 Problem Definitions

In an UNCAPACITATED FACILITY LOCATION (UFL) problem we are given a set of clients  $C$ , a weight function  $w : C \rightarrow \mathbb{N}$  on the clients, a set of facilities  $F$ , an opening cost function  $f : F \rightarrow \mathbb{R}$ , and a distance function  $d : C \times F \rightarrow \mathbb{R}$ . The goal is to find a subset of facilities  $O \subset F$  minimizing

$$\phi_{FL}(C, F, O) = \sum_{c \in C} w(c) \min_{o \in O} \{d(c, o)\} + \sum_{o \in O} f(o) .$$

This problem is uncapacitated in the sense, that any open facility can serve, i.e. be the nearest open facility to, any number of clients. Simply speaking, opening a lot of facilities incurs high opening cost, but small service cost, and vice versa. MUFL is a special case of this problem, where we require the distance function  $d$  to be a metric on  $C \cup F$ .

DKM is a problem closely related to UFL, where we do not differentiate between clients and facilities, but are given a single set of points  $C \subset \mathbb{R}^D$ . We measure distance between points  $p, q \in C$  as  $d(p, q) = \|p - q\|^2$ . Furthermore, instead of imposing an opening cost, we allow at most  $K$  locations to be opened. Hence, the goal is to find  $O \subset C$  with  $|O| = K$  minimizing

$$\phi_{KM}(C, O) = \sum_{c \in C} w(c) \min_{o \in O} \{\|c - o\|^2\} .$$

Notice, that we consider the *weighted* variant of both MUFL and DKM, where each client is associated with a positive weight. Such a weight can be interpreted as the importance of serving the client or as multiple clients present in the same location.

---

\*This is a full version of the paper with the same name that will be presented at CIAC 2017.

## 1.2 Local Search

A popular approach to solving hard problems of combinatorial optimization is local search. The general idea of a local search algorithm is to define a small *neighbourhood* for each feasible solution. Given a problem instance and an initial solution, the algorithm replaces the current solution by a better solution from its neighbourhood. This is repeated until the algorithm finds no improvement, hence has found a solution that is not worse than any solution in its neighbourhood. The runtime and the quality of the produced solutions of a local search algorithm depend heavily on its definition of neighbourhood.

Theoretical aspects of local search are captured in the definition of the complexity class PLS. There is a special type of reduction, called PLS-reduction, with respect to which PLS has complete problems [JHY88]. Notably, there are PLS-complete problems, which exhibit two important properties. First, given an instance and an initial solution, it is PSPACE-complete to find a locally optimal solution computed by a local search started with the given initialization. Second, there is an instance and an initial solution, such that this initial solution is exponentially many local search steps away from every locally optimal solution [MDT10]. There is a stronger version of PLS-reductions, so-called *tight* PLS-reductions which are of special interest, as they preserve both of these properties [PSY90]. PLS-complete problems having these two properties are therefore sometimes called *tightly* PLS-complete.

In the following, we examine a local search algorithm for MUFL und DKM called the *single-swap heuristic*. For MUFL, we allow the algorithm to either close an open facility, newly open a closed facility or do both in one step (*swap* an open facility). Since feasible DKM solutions consist of exactly  $K$  open facilities, we do not allow the algorithm to solely open or close a facility, but only to swap open facilities. Formally, we define these respective neighbourhoods as

$$\begin{aligned} N_{MUFL}(O) &= \{O' \subset F \mid |O \setminus O'| \leq 1 \wedge |O' \setminus O| \leq 1\} \quad \text{and} \\ N_{DKM}(O) &= \{O' \subset C \mid |O \setminus O'| = 1 \wedge |O' \setminus O| = 1\} . \end{aligned}$$

By MUFL/Swap and DKM/Swap we denote the respective problem as a PLS-problem associated with the described single-swap neighbourhood.

## 1.3 Related Work

Approximating MUFL has been subject to considerable amount of research using different algorithmic techniques. The problem can be 4-approximated using LP-rounding [STA97], 3-approximated using a Primal-Dual technique [JV01], and 1.61-approximated using a greedy algorithm [JMS02]. However, it is known that there is no polynomial time algorithm approximating MUFL better than 1.463 unless  $NP \subseteq DTIME(n^{\log \log n})$  [GK99]. Arya et al. showed that the standard local search algorithm of MUFL/Swap computes a 3-approximation for MUFL [AGK<sup>+</sup>04].

A popular generalization of DKM called  $K$ -means admits facilities to be opened anywhere in the  $\mathbb{R}^D$  instead of restricting possible locations to the locations of the clients. The most popular local search algorithm for the  $K$ -means problem is called  $K$ -means algorithm, or Lloyd's algorithm [Llo82]. It is well-known that the solutions produced by the  $K$ -means algorithm can be arbitrarily bad in comparison to an optimal solution. Furthermore, it was shown that in the worst case, the  $K$ -means algorithm requires exponentially many improvement steps to reach a local optimum, even if  $D = 2$  [Vat11]. Recently, Roughgarden and Wang proved that, given a  $K$ -means instance and an initial solution, it is PSPACE-complete to determine the local optimum computed by the  $K$ -means algorithm started on the given initial solution [RW16]. This is in line with several papers proving the same result for the simplex method using different pivoting rules [APR14, FS15]. Kanungo et al. proved that the standard local search algorithm of DKM/Swap computes an  $\mathcal{O}(1)$ -approximation for DKM and hence also for general  $K$ -means [KMN<sup>+</sup>04]. They argue that a variation of the single-swap neighbourhood, where we impose some lower bound on the improvement of a single step, yields an algorithm with polynomial runtime but a slightly worse approximation ratio. However, there is no known upper bound on the runtime of the exact single-swap heuristic, even for unweighted point sets. Another variation of single-swap is the multi-swap heuristic, where we allow the algorithm to simultaneously swap more than one facility in each iteration. For a large enough neighbourhood,

i.e. swapping enough facilities in a single iteration, this heuristic yields a PTAS in Euclidean space with fixed dimension [CAKM16] and in metric spaces with bounded doubling dimension [FRR16].

## 1.4 Our Contribution

In this paper, we analyze the PLS complexity of MUFL/Swap and DKM/Swap. By presenting a tight reduction from MAX 2-SAT, we show that both problems are tightly PLS-complete, hence that both local search algorithms require exponentially many steps in the worst case and that given some initial solution it is PSPACE-complete to find the solution computed by the respective algorithm started on this initial set of open facilities. Our reduction only works for the, previously introduced, weighted variants of MUFL and DKM. That is, we construct instances with a non-trivial weight for each client. Furthermore, our reduction for DKM requires the dimension of the point set to be on the order of the number of points. The performance of the single-swap heuristic is basically unaffected from using the more general variants of MUFL and DKM, since the known approximation bounds also hold for the weighted version of both problems, and since the runtime of the heuristic only depends linearly on the weights and the dimension. However, this means that our reduction is weaker than a proof of the same properties for the unweighted variants or for a constant number of dimensions would be.

**Theorem 1.** *MUFL/Swap and DKM/Swap are tightly PLS-complete.*

We prove the two parts of Theorem 1 in Sections 3 and 4.

## 2 Preliminaries

We present MAX 2-SAT (SAT), a variant of the classic satisfiability problem, which is elementary in the study of PLS. An instance of SAT is a Boolean formula in conjunctive normal form, where each clause consists of exactly 2 literals and has some positive integer weight assigned to it. The cost of a truth assignment is the sum of the weights of all satisfied clauses. The PLS problem SAT/Flip consists of SAT, where the neighbourhood of an assignment is given by all assignments obtained by changing the truth value of a single variable.

**Theorem 2** ([SY91]). *SAT/Flip is tightly PLS-complete.*

For each clause set  $B$  and truth assignment  $T$  we denote the SAT cost of  $T$  with respect to  $B$  by  $w(B, T)$ . For a literal  $x$  we denote the set of all clauses in  $B$  containing  $x$  by  $B(x)$ . Further, we denote the set of all clauses in  $B$  satisfied by  $T$  by  $B_t(T)$  and let  $B_f(T) = B \setminus B_t(T)$ . Finally, we set  $w_{max}^B = \max_{b \in B} \{w(b)\}$ .

## 3 The Facility Location Reduction

In the following, we formulate and prove one of our main results.

**Proposition 3.** *SAT/Flip  $\leq_{PLS}$  MUFL/Swap and this reduction is tight.*

The following proof of Proposition 3 is divided into three parts. First, we present our construction of a PLS-reduction  $(\Phi, \Psi)$ , second, we argue on the correctness of this reduction and finally we show that the reduction is tight.

### 3.1 Construction of $\Phi$ and $\Psi$

First, we construct the function  $\Phi$  mapping an instance  $(B, w) \in \text{MAX 2-SAT}$  over the variables  $\{x_n\}_{n \in [N]}$  to an instance  $(C, \omega, F, f, d) \in \text{METRIC UNCAPACITATED FACILITY LOCATION}$ . In the following, we denote  $M := |B|$ . Each variable  $x_n$  appears as a facility twice, once as a positive and once as a negative literal. Formally, we set  $F = \{x_n, \bar{x}_n\}_{n \in [N]}$ . We further locate a client at

each facility and a client corresponding to each clause, so  $C = F \cup B$ . We set the distance function  $d : C \cup F \times C \cup F \rightarrow \mathbb{R}$  to

$$d(p, q) = d(q, p) = \begin{cases} 0 & \text{if } p = q \\ 1 & \text{if } p = x_n \wedge q = \bar{x}_n \\ \frac{4}{3} & \text{if } (p = x_n \vee p = \bar{x}_n) \wedge q = b_m \wedge p \in b_m \\ \frac{5}{3} & \text{if } (p = x_n \vee p = \bar{x}_n) \wedge q = b_m \wedge \bar{p} \in b_m \\ 2 & \text{else.} \end{cases}$$

Simply speaking, a literal has distance 1 from its negation, clauses have distance  $4/3$  from literals they contain, distance  $5/3$  from literals whose negation they contain, and all other clients/facilities have distance 2 from each other. It is easy to see that  $d$  is a metric. The weight of a client corresponding to a clause is the same as the weight of the clause. If a client corresponds to a literal, then its weight is  $W = M \cdot w_{max}^B$ .

$$\omega(p) = \begin{cases} w(b_m) & \text{if } p = b_m \\ W & \text{else} \end{cases}$$

The opening cost function is constant  $f \equiv 2W$ .

Second, we construct the function  $\Psi$  mapping solutions of  $\Phi(B, w)$  back to solutions of  $(B, w)$ . Given a set  $O \subset F$  we let each variable  $x_n$  be true if the facility  $x_n \in O$  and let it be false otherwise.

In the following, we denote  $\Phi(B, w) = (C, \omega, F, 2W, d)$ ,  $\Psi(B, w, O) = T_O$ , and  $d(c, O) = \min_{o \in O} \{d(c, o)\}$ .

### 3.2 $(\Phi, \Psi)$ is a PLS-reduction

To prove that  $(\Phi, \Psi)$  is a PLS-reduction we need to argue that  $T_O$  is locally optimal for  $(B, w)$  if  $O$  is locally optimal for  $\Phi(B, w)$ . Observe, that  $\Psi$  is not injective, since  $\Phi(B, w)$  has more feasible solutions than  $(B, w)$ . We can tackle this problem by characterizing a subset of solutions for  $\Phi(B, w)$  we call *reasonable* solutions.

**Definition 4.** Let  $O \subset F$ . We call  $O$  reasonable if  $|O| = N$  and

$$\forall n \in [N] : x_n \in O \vee \bar{x}_n \in O .$$

Reasonable solutions have several useful properties, which we prove in the following. The restriction of  $\Psi$  to reasonable solutions is a bijection, the MUFL cost of a reasonable solution is closely related to the SAT cost of its image under  $\Psi$ , and all locally optimal solutions of  $\Phi(B, w)$  are reasonable. This characterization of solutions is crucial to proving correctness and tightness of our reduction.

**Lemma 5.** If  $O, O' \subset F$  are reasonable solutions for  $\Phi(B, w)$ , then

$$w(B, T_O) < w(B, T_{O'}) \Leftrightarrow \phi_{FL}(C, F, O) > \phi_{FL}(C, F, O') .$$

*Proof.* The following claim is essential to our proof of Lemma 5.

**Claim 6.** If  $O \subset F$  is reasonable, then

$$\phi_{FL}(C, F, O) = \frac{4}{3} \sum_{b_m \in B_t(T_O)} w(b_m) + \frac{5}{3} \sum_{b_m \in B_f(T_O)} w(b_m) + 3WN .$$

*Proof.* Since  $|O| = N$ , we have that the total opening cost of facilities is  $2WN$ . Observe, that since either  $x_n$  or  $\bar{x}_n$  is in  $O$ , we further obtain that the total service cost of all clients  $\{x_n, \bar{x}_n\}_{n \in [N]}$  is  $WN$ . Similar to before, we can observe a one-to-one mapping of the truth assignment of a variable, to whether the corresponding positive or negative literal is in  $O$ . It is easy to see that the clients corresponding to a clause in  $B_t(T_O)$  have at least one open facility at distance  $4/3$ , while the clients corresponding to a clause in  $B_f(T_O)$  have two facilities at distance  $5/3$  and the rest at distance 2.  $\square$

For the sake of brevity we introduce the notation

$$B_{ab} = B_a(T_O) \cap B_b(T_{O'})$$

for  $a, b \in \{t, f\}$ . Observe that

$$w(B, T_O) < w(B, T_{O'}) \Leftrightarrow \sum_{b_m \in B_{tf}} w(b_m) < \sum_{b_m \in B_{ft}} w(b_m) . \quad (1)$$

Hence, using Lemma 6 we obtain

$$\begin{aligned} \phi_{FL}(C, F, O') &= 3WN + \frac{4}{3} \sum_{b_m \in B_t(T_{O'})} w(b_m) + \frac{5}{3} \sum_{b_m \in B_f(T_{O'})} w(b_m) \\ &= 3WN + \frac{4}{3} \sum_{b_m \in B_{tt}} w(b_m) + \frac{4}{3} \sum_{b_m \in B_{ft}} w(b_m) + \\ &\quad \frac{5}{3} \sum_{b_m \in B_{tf}} w(b_m) + \frac{5}{3} \sum_{b_m \in B_{ff}} w(b_m) \\ &\stackrel{(1)}{<} 3WN + \frac{4}{3} \sum_{b_m \in B_{tt}} w(b_m) + \frac{5}{3} \sum_{b_m \in B_{ft}} w(b_m) + \\ &\quad \frac{4}{3} \sum_{b_m \in B_{tf}} w(b_m) + \frac{5}{3} \sum_{b_m \in B_{ff}} w(b_m) \\ &= 3WN + \frac{4}{3} \sum_{b_m \in B_t(T_O)} w(b_m) + \sum_{b_m \in B_f(T_O)} w(b_m) = \phi_{FL}(C, F, O) \end{aligned}$$

□

**Lemma 7.** *If  $O \subset F$  is a locally optimal solution for  $\Phi(B, w)$ , then  $O$  is reasonable.*

A detailed proof of Lemma 7 can be found in Section 3.3. We can combine these results to obtain the correctness of our reduction.

**Corollary 8.** *If  $O$  is locally optimal for  $\Phi(B, w)$ , then  $T_O$  is locally optimal for  $(B, w)$ .*

*Proof.* Assume to the contrary that  $T_O$  is not locally optimal. If  $O$  is not reasonable, then it is not locally optimal by Lemma 7. Therefore, assume that  $O$  is reasonable. Since  $T_O$  is not locally optimal, we know that there exists an  $n \in [N]$ , such that  $w(B, T_O^{\bar{n}}) > w(B, T_O)$ , where  $T_O^{\bar{n}}$  denotes  $T_O$  with an inverted assignment of the  $n^{\text{th}}$  variable. Since  $O^{\bar{n}} := (O \setminus \{x_n\}) \cup \{\bar{x}_n\}$  is reasonable,  $\Psi(B, w, O^{\bar{n}}) = T_O^{\bar{n}}$  and by Lemma 5 we know that

$$\phi_{FL}(C, F, O^{\bar{n}}) < \phi_{FL}(C, F, O) ,$$

and hence can conclude that  $O$  is not locally optimal. □

### 3.3 Proof of Lemma 7

The following proof of Lemma 7 is presented in two steps. First, we argue in Lemma 9 that no locally optimal solution can contain both a literal and its negation. Second, we show in Lemma 10 that every locally optimal solution contains a facility corresponding to each of the variables. Combining these two results gives us Lemma 7 as a corollary. From the following results we can moreover conclude that once the single-swap algorithm has reached a reasonable solution, it will always stay at a reasonable solution. We take up on this fact in Section 3.4, where we argue on the tightness of our reduction.

**Lemma 9.** *If  $x_n, \bar{x}_n \in O$ , then  $O$  is not locally optimal.*

*Proof.* We show that closing the facility located at  $x_n$  strictly decreases the cost, and hence that  $O$  can not be locally optimal. When closing the facility  $x_n$ , we have to let all clients previously served by this facility (including the client located at  $x_n$ ) be served by another facility. Choosing  $\bar{x}_n$  as the replacement, we do not increase the cost by too much. More specifically, we can pay the additional cost with the cost we save from not opening  $x_n$ . Recall, that  $B(x_n)$  is the set of all clauses containing the literal  $x_n$ , hence that  $|B(x_n)| \leq M$ . Observe, that no client in  $C \setminus B(x_n)$  (except  $x_n$ ) is closer to  $x_n$  than it is to  $\bar{x}_n$ . We obtain

$$\begin{aligned} \phi_{FL}(C, F, O) &= \sum_{\substack{c \in C \setminus B(x_n) \\ c \neq x_n}} \omega(c)d(c, O) + \sum_{b_m \in B(x_n)} \omega(b_m) \frac{4}{3} + |O| 2W \\ &> \sum_{\substack{c \in C \setminus B(x_n) \\ c \neq x_n}} \omega(c)d(c, O) + \sum_{b_m \in B(x_n)} \omega(b_m) \frac{5}{3} + W + (|O| - 1)2W \\ &\geq \phi_{FL}(C, F, O \setminus \{x_n\}) . \end{aligned}$$

□

**Lemma 10.** *If  $x_n, \bar{x}_n \notin O$ , then  $O$  is not locally optimal.*

*Proof.* Similar to before, we show that opening a facility at  $x_n$  strictly decreases the cost. When opening the facility at  $x_n$  we have to save enough service cost by serving locations from it, that we can pay for opening the facility. Connecting the clients located at  $x_n$  and  $\bar{x}_n$  to the newly opened facility is sufficient. We obtain

$$\begin{aligned} \phi_{FL}(C, F, O) &= \sum_{c \in C \setminus \{x_n, \bar{x}_n\}} \omega(c)d(c, O) + \underbrace{\sum_{c \in \{x_n, \bar{x}_n\}} \omega(c)d(c, O)}_{=4W} + |O| 2W \\ &> \sum_{c \in C \setminus \{x_n, \bar{x}_n\}} \omega(c)d(c, O) + W + (|O| + 1)2W \\ &\geq \phi_{FL}(C, F, O \cup \{x_n\}) . \end{aligned}$$

□

### 3.4 $(\Phi, \Psi)$ is a Tight Reduction

We show that  $(\Phi, \Psi)$  is a tight reduction by only considering its behaviour on reasonable solutions. Lemma 7 tells us that restricted to reasonable solutions, the single-swap local search behaves on  $\Phi(B, w)$  exactly the same as the flip local search behaves on  $(B, w)$ . Additionally, we use the fact that once single-swap has reached a reasonable solution, it will always stay at a reasonable solution. Formally, we need to find a set of feasible solutions  $\mathcal{R}$  for  $(C, \omega, F, 2W, d)$ , such that

1.  $\mathcal{R}$  contains all local optima.
2. for every feasible solution  $T$  of  $(B, w)$ , we can compute  $O \in \mathcal{R}$  with  $T_O = T$  in polynomial time.
3. if the transition graph  $TG(C, \omega, F, 2W, d)$  contains a directed path  $O \rightsquigarrow O'$ , with  $O, O' \in \mathcal{R}$  but all internal path vertices outside of  $\mathcal{R}$ , then  $TG(B, w)$  contains the edge  $(T_O, T_{O'})$  or  $T_O = T_{O'}$ .

Let  $\mathcal{R}$  be the set of all reasonable solutions.  $\mathcal{R}$  contains all local optima of  $(C, \omega, F, 2W, d)$ , by Lemma 7. The restriction of  $\Psi$  to  $\mathcal{R}$  is bijective and we can obviously compute the inverse in polynomial time. To prove the final property of tight reductions, we use the following result, which is a byproduct of the proof of Lemma 7.

**Corollary 11.** *If  $O \in \mathcal{R}$  and  $O' \notin \mathcal{R}$ , then  $(O, O') \notin TG(C, \omega, F, 2W, d)$ .*

Assume  $O \rightsquigarrow O'$  is a directed path in  $TG(C, \omega, F, 2W, d)$ , with  $O, O' \in \mathcal{R}$  but all internal path vertices outside of  $\mathcal{R}$ . By Corollary 11, this path consists of the single edge  $(O, O')$ . This means that  $\phi_{FL}(C, F, O) > \phi_{FL}(C, F, O')$  and thus, by Lemma 5, we obtain  $w(B, T_O) < w(B, T_{O'})$ . Hence, we conclude the tightness proof by observing that  $(T_O, T_{O'}) \in TG(B, w)$ .

## 4 The $K$ -Means Reduction

We complement our results by showing that we can obtain tight PLS-completeness for DKM/Swap, as well.

**Proposition 12.** *SAT/Flip  $\leq_{PLS}$  DKM/Swap and this reduction is tight.*

To prove Proposition 12, we can basically use the reduction presented in Section 3.1. We need to change some of the constants involved in the construction to make sure that we find a set of points in  $\mathbb{R}^D$  with the required interpoint distances. However, the general approach stays the same and we obtain essentially the same intermediate results. In the following, we will point out the differences in the construction of  $(\Phi, \Psi)$  and indicate which proofs require adjustments. After proving the hardness result based on the abstract definition of  $C$ , we show that there is indeed a point set in  $\mathbb{R}^D$  exhibiting the required squared euclidean distances.

### 4.1 Modifications to $(\Phi, \Psi)$

As before, let  $(B, w)$  be a MAX 2-SAT instance over the variables  $\{x_n\}_{n \in [N]}$ . We construct an instance  $(C, \omega, K) \in \text{DISCRETE } K\text{-MEANS}$ . Abstractly define the point set  $C = \{x_n, \bar{x}_n\}_{n \in [N]} \cup B$ . The distance function  $d : C \times C \rightarrow \mathbb{R}$  is similar to before

$$d(p, q) = d(q, p) = \begin{cases} 0 & \text{if } p = q \\ 1 & \text{if } p = x_n \wedge q = \bar{x}_n \\ 1 + \epsilon & \text{if } (p = x_n \vee p = \bar{x}_n) \wedge q = b_m \wedge p \in b_m \\ 1 + c\epsilon & \text{if } (p = x_n \vee p = \bar{x}_n) \wedge q = b_m \wedge \bar{p} \in b_m \\ 1 + 2\epsilon & \text{else,} \end{cases}$$

where  $1 < c < 2$  and

$$\epsilon = \frac{1}{4N + 2M}.$$

While the distances are scaled in comparison to the MUFL reduction, the central structure remains unchanged. The points closest to each other are literals and their negation. Clauses are closer to literals they contain, than to the literal's negation. All other point pairs have the same, even larger, distance to each other.

The weight function remains unchanged. That is, the weight of a point corresponding to a clause is the SAT weight of the clause, the weight of a point corresponding to a (negated) variable is  $W = M \cdot w_{max}^B$ . Finally, we choose  $K = N$ . Like the weight function,  $\Psi$  remains unchanged. We denote  $\Phi(B, w) = (C, \omega, N)$ .

### 4.2 Correctness of the DKM Reduction

Just as before, we have the problem that  $\Psi$  is not injective. However, we can again solve the problem using the previously introduced notion of reasonable solutions. While the first condition ( $|O| = N$ ) is trivially fulfilled, we utilize the second property to ensure that  $\Psi$  becomes a bijection when being restricted to reasonable solutions. Moreover, we obtain analog results to Lemma 5 and 7.

**Lemma 13.** *If  $O, O' \subset C$  are reasonable solutions for  $\Phi(B, w)$ , then*

$$w(B, T_O) < w(B, T_{O'}) \Leftrightarrow \phi_{KM}(C, O) > \phi_{KM}(C, O').$$

*Proof.* First, we proof a claim analog to Claim 6.

**Claim 14.** *If  $O \subset C$  is reasonable, then*

$$\phi_{KM}(C, O) = NW + (1 + \epsilon) \sum_{b_m \in B_t(X_C)} w(b_m) + (1 + c\epsilon) \sum_{b_m \in B_f(X_C)} w(b_m) .$$

*Proof.* We have that  $(T_O)_n = 1$  if  $x_n \in O$  and  $(T_O)_n = 0$  if  $\bar{x}_n \in O$ . Simply speaking, there is a one-to-one mapping of the truth assignment of a variable, to whether the corresponding positive or negative point is part of the solution. We obtain that  $\phi_{KM}(\{x_n, \bar{x}_n\}_{n \in [N]}, O) = NW$ , since each point corresponding to a literal is either in  $O$  and has cost 0, or its negated literal at distance 1 is in  $O$  and it has cost  $W$ . It is easy to see, by definition of the point set and  $\Psi$ , that the points corresponding to a clause in  $B_t(X_C)$  have at least one mean at distance  $1 + \epsilon$  and that the points corresponding to a clause in  $B_f(X_C)$  have two means at distance  $1 + c\epsilon$  and the rest at distance  $1 + 2\epsilon$ .  $\square$

The subsequent argument is analog to the proof presented for Lemma 5.  $\square$

Almost all of the additional work required for the DKM correctness goes into the proof of the following lemma.

**Lemma 15.** *If  $O \subset C$  is a locally optimal solution for  $\Phi(B, w)$ , then  $O$  is reasonable.*

Here, we have to ensure that locally optimal solutions do not contain points corresponding to clauses. This was not an issue in the MUFL proof, since clauses are not available for opening in that case.

Using these intermediate results we can see that this is a tight reduction following the same arguments presented in Section 3.4

### 4.3 Proof of Lemma 15

Observe, that each point  $b_m \in C$  has exactly two points at distance  $1 + \epsilon$  and two points at distance  $1 + c\epsilon$  (the points corresponding to the literals in the clause  $b_m$  and their negations, respectively). In the following, we call these four points *adjacent* to  $b_m$ . All the other points have distance  $1 + 2\epsilon$  to  $b_m$  and are hence strictly farther away. Assume to the contrary that there exists an  $n \in [N]$ , such that  $x_n, \bar{x}_n \notin O$ .

*Case 1:* There exists an  $m \in [M] : b_m \in O$ , such that  $b_m = \{x_o, x_p\}$  (where one or both of these literals might be negated). One important observation is that if we exchange  $b_m$  for some other location then only its own cost and the cost of its adjacent points can increase. All other points, which might be connected to  $b_m$ , are at distance  $1 + 2\epsilon$  and can hence be connected to any other location for at most the same cost.

*Case 1.1:*  $x_o, \bar{x}_o, x_p, \bar{x}_p \notin O$ . Each point adjacent to  $b_m$  has weight  $W$  and has distance at least  $1 + \epsilon$  to every other points in  $P$ . Hence, we have that  $\phi(\{b_m, x_o, \bar{x}_o, x_p, \bar{x}_p\}, O) \geq (4 + 4\epsilon)W$ . However,

$$\begin{aligned} \phi(\{b_m, x_o, \bar{x}_o, x_p, \bar{x}_p\}, \{x_o\}) &\leq (1 + c\epsilon)\omega(b_m) + W + (2 + 4\epsilon)W \\ &< (4 + 4\epsilon)W , \end{aligned}$$

and hence  $(O \setminus \{b_m\}) \cup \{x_o\}$  is in the neighbourhood of  $O$  and has strictly smaller cost.

*Case 1.2:*  $x_p \in O \vee \bar{x}_p \in O$  and  $x_o, \bar{x}_o \notin O$ . In this case, removing  $b_m$  from  $O$  does not affect the cost of  $x_p$  and  $\bar{x}_p$ . We obtain  $\phi(\{b_m, x_o, \bar{x}_o\}, O) \geq (2 + 2\epsilon)W$ . Observe, that

$$\phi(\{b_m, x_o, \bar{x}_o\}, (O \setminus \{b_m\}) \cup \{x_o\}) \leq (1 + c\epsilon)\omega(b_m) + W < 2W .$$

*Case 1.3:*  $x_p \in O \vee \bar{x}_p \in O$  and  $x_o \in O \vee \bar{x}_o \in O$ . Here we have that removing  $b_m$  from  $O$  does not affect the cost of its adjacent points at all. However, similar to before we have  $\phi(\{b_m, x_n, \bar{x}_n\}, O) \geq (2 + 2\epsilon)W$ . Again, we obtain

$$\phi(\{b_m, x_n, \bar{x}_n\}, (C \setminus \{b_m\}) \cup \{x_n\}) \leq (1 + c\epsilon)\omega(b_m) + W < 2W .$$



*Case 2:* There is no  $m \in [M]$ , such that  $b_m \in O$ . Consequently, there is an  $o \in [N], o \neq n : x_o, \bar{x}_o \in O$ . W.l.o.g. assume that  $|B(x_o)| < M$  (otherwise just exchange  $x_o$  for  $\bar{x}_o$  in the following argument). Observe that

$$\phi(B(x_o) \cup \{x_o, x_n, \bar{x}_n\}, O) = (2 + 4\epsilon)W + (1 + \epsilon) \sum_{b_m \in B(x_o)} \omega(b_m) .$$

The only points affected by removing  $x_o$  from  $O$  are  $x_o$  and the points corresponding to clauses in  $B(x_o)$ . Hence,

$$\begin{aligned} \phi(C \setminus (B(x_o) \cup \{x_o, x_n, \bar{x}_n\}), O) &= \phi(C \setminus (B(x_o) \cup \{x_o, x_n, \bar{x}_n\}), O \setminus \{x_o\}) \\ &\geq \phi(C \setminus (B(x_o) \cup \{x_o, x_n, \bar{x}_n\}), (O \setminus \{x_o\}) \cup \{x_n\}) . \end{aligned}$$

However, recall that the points in  $B(x_o)$  are at distance  $(1 + c\epsilon)$  from  $\bar{x}_o \in O$ . We obtain

$$\begin{aligned} &\phi(B(x_o) \cup \{x_o, x_n, \bar{x}_n\}, (O \setminus \{x_o\}) \cup \{x_n\}) \\ &\leq \phi(B(x_o) \cup \{x_o, \bar{x}_n\}, \{\bar{x}_o, x_n\}) \\ &= 2W + (1 + \epsilon) \sum_{b_m \in B(x_o)} \omega(b_m) + ((c - 1)\epsilon) \sum_{b_m \in B(x_o)} \omega(b_m) \\ &< 2W + (1 + \epsilon) \sum_{b_m \in B(x_o)} \omega(b_m) + \epsilon W \\ &< (2 + 4\epsilon)W + (1 + \epsilon) \sum_{b_m \in B(x_o)} \omega(b_m) \\ &= \phi(B(x_o) \cup \{x_o, x_n, \bar{x}_n\}, O) . \end{aligned}$$

□

#### 4.4 Embedding $C$ into $\ell_2^2$

So far, we regarded  $C$  as an abstract point set, only given by fixed pairwise interpoint distances. We show that there is an isometric embedding of  $C$  into  $\ell_2^2$ , that is, a set of points in  $\mathbb{R}^D$  exhibiting exactly these interpoint distances as squared Euclidean distance. In the following, we denote by  $\mathbf{1}_D$  the  $D$ -dimensional vector, where each entry is 1, and by  $\delta_{ij}$  the Kronecker delta.

**Theorem 16** ([Sch38]). *A distance matrix  $M \in \mathbb{R}^{N \times N}$  can be embedded into  $\ell_2^2$  if and only if*

$$\forall u \in \mathbb{R}^N \text{ with } u \cdot \mathbf{1}_N = 0 \text{ we have } u^T M u \leq 0 .$$

In the following let  $M_C$  be the matrix corresponding to the point set  $C$ . That is, we chose some ordering of the point set  $C = \{c_1, \dots, c_{2N+M}\}$  and set  $(M_C)_{i,j} = d(c_i, c_j)$ . Observe, that

$$(M_C)_{i,j} = 1 - \delta_{ij} + (d(c_i, c_j) - 1)(1 - \delta_{ij}) ,$$

where the second summand is always non-negative.

**Lemma 17.**  *$M_C$  can be embedded into  $\ell_2^2$ .*

*Proof.* Let  $u \in \mathbb{R}^{2N+M}$  with  $u \cdot \mathbf{1}_{2N+M} = 0$ . By Theorem 16, it suffices to show

$$\begin{aligned} u^T M_C u &= \sum_{i,j} (M_C)_{i,j} u_i u_j \\ &= \sum_{i,j} u_i u_j - \sum_{i,j} u_i u_j \delta_{ij} + \sum_{i,j} (d(c_i, c_j) - 1) u_i u_j (1 - \delta_{ij}) \\ &= \underbrace{\left( \sum_i u_i \right)^2}_{=0} - \sum_i u_i^2 + \sum_{i,j} (d(c_i, c_j) - 1) u_i u_j (1 - \delta_{ij}) \end{aligned}$$

$$\begin{aligned}
 &\leq -\|u\|^2 + \sum_{i,j} (d(c_i, c_j) - 1) |u_i| |u_j| (1 - \delta_{ij}) \\
 &\leq -\|u\|^2 + 2\epsilon \sum_{i,j} |u_i| |u_j| \\
 &= -\|u\|^2 + 2\epsilon \left( \sum_i |u_i| \right)^2 \\
 &\leq -\|u\|^2 + 2\epsilon(2N + M) \|u\|^2 = 0,
 \end{aligned}$$

where the second to last inequality holds by Cauchy-Schwarz.  $\square$

**Theorem 18** ([Tor52]). *If  $M$  is a distance matrix embeddable into  $\ell_2^2$ , then there is a polynomial-time algorithm that computes a matrix  $P$  whose rows form a set  $\{p_n\}_{n \in [N]}$  with  $M_{i,j} = \|p_i - p_j\|^2$ .*

## 5 Application to Fuzzy $K$ -Means

Clustering problems, such as DKM, appear in many applications of machine learning and data mining and are closely related to facility location problems. Problems like DKM, where each point is assigned to a single location, are sometimes called *hard clustering* problems. If we allow clusters to overlap, so that a point can be assigned to multiple locations, then we speak of a *soft* clustering. One popular soft clustering generalization of the  $K$ -means problem is the *fuzzy  $K$ -means* problem. In addition to the  $K$  location vectors, the fuzzy  $K$ -means problem seeks for a set of *memberships* assigning some fraction of each point to each location. Formally, the goal of the DISCRETE FUZZY  $K$ -MEANS (DFKM) problem, given  $C \subset \mathbb{R}^D$  and  $K \in \mathbb{N}$ , is to find  $O \subset C$  and  $r : C \times O \rightarrow \mathbb{R}_{\geq 0}$  minimizing

$$\phi_{FKM}(C, O, r) = \sum_{c \in C} \sum_{o \in O} r(c, o)^2 \|c - o\|^2,$$

subject to  $\forall c \in C : \sum_{o \in O} r(c, o) = 1$ .

For each fixed set of locations  $O \subset \mathbb{R}^D$  we can compute a membership function  $r$  minimizing  $\phi_{FKM}(C, O, r)$  in polynomial time [Dun73]. Hence, we obtain that DFKM/Swap is a PLS problem. So far, there are no known results on the quality of the solutions produced by the standard local search algorithm of DFKM/Swap. The reduction presented for DKM/Swap can be generalized to apply to DFKM/Swap, as well.

**Theorem 19.** *DFKM/Swap is tightly PLS-complete.*

We prove Theorem 19 by presenting a tight PLS reduction of DFKM/Swap to POS NAE MAX 2-SAT (PNAESAT)/Flip, a variant of the previously introduced SAT/Flip.

### 5.1 Preliminaries

An instance of PNAESAT is a weighted Boolean formula in conjunctive normal form, where each clause consists of 2 *positive* literals, and the cost of a truth assignment is given by the sum over the weights of all clauses whose two variables differ in their truth value. As before, in the PLS problem PNAESAT/Flip, the neighbourhood of an assignment is given by all assignments obtained by changing the truth value of a single variable. For each clause set  $B$  and truth assignment  $T$  we denote the NAE cost of  $T$  with respect to  $B$  by  $w_{NAE}(B, T)$ .

**Theorem 20** ([SY91]). *PNAESAT/Flip is tightly PLS-complete.*

**Proposition 21.** *PNAESAT/Flip  $\leq_{PLS}$  DFKM/Swap and this reduction is tight.*

The following proof of Proposition 21 will basically use the same reduction previously presented for DKM/Swap. However, first we need to modify the given PNAESAT instance slightly, and change some of the constants involved.

## 5.2 Modification to $(B, w)$

As before, let  $(B = \{b_m\}_{m \in [M]}, w)$  be a PNAESAT instance over the variables  $\{x_n\}_{n \in [N]}$ . From  $B$  we construct a new set of clauses  $B'$  which will be the input to our reduction. For each clause  $b_m = \{x_o, x_p\} \in B$   $B'$  contains the two clauses

$$b_m^1 = \{x_o, x_p\} \text{ and } b_m^2 = \{\bar{x}_o, \bar{x}_p\}.$$

We define our reduction function based on  $(B', w)$ . We still denote  $w_{max}^B = \max_{m \in [M]} \{w(b_m)\}$ , but redefine  $M = |B'|$ .

## 5.3 Construction of $\Phi$ and $\Psi$

Given  $(B', w)$ , we construct an instance  $(C', \omega, K) \in \text{DISCRETE FUZZY } K\text{-MEANS}$ . As before, abstractly define the point set  $C' = \{x_n, \bar{x}_n\}_{n \in [N]} \cup B$ . The distance function  $d : C \times C \rightarrow \mathbb{R}$  is again

$$d(p, q) = d(q, p) = \begin{cases} 0 & \text{if } p = q \\ 1 & \text{if } p = x_n \wedge q = \bar{x}_n \\ 1 + \epsilon & \text{if } (p = x_n \vee p = \bar{x}_n) \wedge q = b_m \wedge p \in b_m \\ 1 + c\epsilon & \text{if } (p = x_n \vee p = \bar{x}_n) \wedge q = b_m \wedge \bar{p} \in b_m \\ 1 + 2\epsilon & \text{else,} \end{cases}$$

where  $1 < c < 2$ . However, we set

$$\epsilon = \min \left\{ \frac{1}{4N + 2M}, \frac{M - 1}{9N^2M} \right\}.$$

Let the weight function  $\omega$  be defined as before

$$\omega(c) = \begin{cases} w(b_m) & \text{if } c = b_m^i \\ W & \text{else,} \end{cases}$$

however we choose  $W = 4N^2 \cdot M \cdot w_{max}^B$ . As before, let  $K = N$ . The function  $\Psi$  remains unchanged.

## 5.4 Properties of $(C', \omega, N)$

Recall the following important properties of the fuzzy  $K$ -means objective function.

**Lemma 22** ([Dun73]). *Let  $C \subset \mathbb{R}^D$  and fix any set of means  $O \subset \mathbb{R}^D$ . For each  $c \in C$  and  $o \in O$  we have that the optimal membership of  $c$  to the mean  $o$  is given by*

$$r(c, o) = \frac{\|c - o\|^{-2}}{\sum_{o' \in O} \|c - o'\|^{-2}}.$$

*Substituting for all optimal memberships we obtain*

$$\phi_{FKM}(C, O) = \sum_{c \in C \setminus O} \frac{\omega(c)}{\sum_{o \in O} \|c - o\|^{-2}}.$$

**Lemma 23.** *For all  $O \subset C'$  with  $|O| = N$  we have*

$$\forall c \in C' \setminus O \forall o \in O : r(c, o) > \frac{1}{2N}.$$

*Proof.* By definition of the interpoint distances in  $C'$  we obtain

$$r(c, o) = \frac{\|c - o\|^{-2}}{\sum_{o' \in O} \|c - o'\|^{-2}} \geq \frac{(1 + 2\epsilon)^{-1}}{|O|} > \frac{1}{2N}.$$

□

### 5.5 $(\Phi, \Psi)$ is a PLS-Reduction

**Lemma 24.** *If  $O \subset C'$  is reasonable, then*

$$\phi_{FKM}(C', O) = \frac{N + N2\epsilon}{N + 2\epsilon} + 2\Gamma_2 \sum_{b_m \in B_t(T_O)} w(b_m) + (\Gamma_1 + \Gamma_3) \sum_{b_m \in B_f(T_O)} w(b_m),$$

where

$$\Gamma_1 = \frac{1}{\frac{N-2}{1+2\epsilon} + \frac{2}{1+\epsilon}}, \quad \Gamma_2 = \frac{1}{\frac{N-2}{1+2\epsilon} + \frac{1}{1+\epsilon} + \frac{1}{1+c\epsilon}}, \quad \text{and} \quad \Gamma_3 = \frac{1}{\frac{N-2}{1+2\epsilon} + \frac{2}{1+c\epsilon}}.$$

*Proof.* We have that  $(T_O)_n = 1$  if  $x_n \in C$  and  $(T_O)_n = 0$  if  $\bar{x}_n \in O$ . Simply speaking, there is a one-to-one mapping of the truth assignment of a variable, to whether the corresponding positive or negative point is part of the solution. We obtain that  $\phi_{FKM}(\{x_n, \bar{x}_n\}_{n \in [N]}, O) = \frac{N+N2\epsilon}{N+2\epsilon}$ , since each point corresponding to a literal is either in  $O$  and has cost 0, or it has its negated literal at distance 1 and  $N-1$  means at distance  $1+2\epsilon$  and hence has cost

$$\frac{1}{\frac{N-1}{1+2\epsilon} + 1} = \frac{1+2\epsilon}{N+2\epsilon}.$$

Recall, that a clause of PNAESAT is satisfied if one variable evaluates to true, and one to false. Hence, the points  $b_m^1$  and  $b_m^2$  corresponding to a clause in  $b_m \in B_t(T_O)$  have one mean at distance  $1+\epsilon$ , one mean at distance  $1+c\epsilon$  and  $N-2$  means at distance  $1+2\epsilon$ . We obtain, that  $\forall b_m \in B_t(T_O) : \phi_{FKM}(\{b_m^1, b_m^2\}, O) = 2w(b_m) / \left( \frac{N-2}{1+2\epsilon} + \frac{1}{1+\epsilon} + \frac{1}{1+c\epsilon} \right)$ . Conversely, the points  $b_m^1$  and  $b_m^2$  corresponding to a clause in  $B_f(T_O)$  split in two different groups. One of them has two means at distance  $1+\epsilon$  and the other has two means at distance  $1+c\epsilon$ , while both have  $N-2$  means at distance  $1+2\epsilon$ . We obtain, that  $\forall b_m \in B_f(T_O) : \phi_{FKM}(\{b_m^1, b_m^2\}, O) = w(b_m) / \left( \frac{N-2}{1+2\epsilon} + \frac{2}{1+\epsilon} \right) + w(b_m) / \left( \frac{N-2}{1+2\epsilon} + \frac{2}{1+c\epsilon} \right)$ .  $\square$

**Lemma 25.** *If  $O, O' \subset C'$  are reasonable, then*

$$w_{NAE}(B, T_O) < w_{NAE}(B, T_{O'}) \Leftrightarrow \phi_{FKM}(C', O) > \phi_{FKM}(C', O').$$

*Proof.* Observe that

$$w(B, T_O) < w(B, T_{O'}) \Leftrightarrow \sum_{b_m \in B_{tf}} w(b_m) < \sum_{b_m \in B_{ft}} w(b_m), \quad (2)$$

and

$$\begin{aligned} \Gamma_1 + \Gamma_3 - 2\Gamma_2 &= \frac{1}{\frac{N-2}{1+2\epsilon} + \frac{2}{1+\epsilon}} + \frac{1}{\frac{N-2}{1+2\epsilon} + \frac{2}{1+c\epsilon}} - \frac{2}{\frac{N-2}{1+2\epsilon} + \frac{1}{1+\epsilon} + \frac{1}{1+c\epsilon}} \\ &= \frac{2 \left( \frac{1}{1+c\epsilon} - \frac{1}{1+\epsilon} \right)^2}{\left( \frac{N-2}{1+2\epsilon} + \frac{2}{1+\epsilon} \right) \left( \frac{N-2}{1+2\epsilon} + \frac{2}{1+c\epsilon} \right) \left( \frac{N-2}{1+2\epsilon} + \frac{1}{1+\epsilon} + \frac{1}{1+c\epsilon} \right)} > 0. \end{aligned} \quad (3)$$

Hence, using Lemma 24 we obtain

$$\begin{aligned} \phi_{FKM}(C', T_{O'}) &= \frac{N + N2\epsilon}{N + 2\epsilon} + 2\Gamma_2 \sum_{b_m \in B_t(T_{O'})} w(b_m) + \\ &\quad (\Gamma_1 + \Gamma_3) \sum_{b_m \in B_f(T_{O'})} w(b_m) \\ &= \frac{N + N2\epsilon}{N + 2\epsilon} + 2\Gamma_2 \sum_{b_m \in B_{tt}} w(b_m) + 2\Gamma_2 \sum_{b_m \in B_{ft}} w(b_m) + \\ &\quad (\Gamma_1 + \Gamma_3) \sum_{b_m \in B_{tf}} w(b_m) + (\Gamma_1 + \Gamma_3) \sum_{b_m \in B_{ff}} w(b_m) \end{aligned}$$

$$\begin{aligned}
 & \stackrel{(2),(3)}{<} \frac{N + N2\epsilon}{N + 2\epsilon} + 2\Gamma_2 \sum_{b_m \in B_{tt}} w(b_m) + (\Gamma_1 + \Gamma_2) \sum_{b_m \in B_{ft}} w(b_m) + \\
 & \quad 2\Gamma_2 \sum_{b_m \in B_{tf}} w(b_m) + (\Gamma_1 + \Gamma_3) \sum_{b_m \in B_{ff}} w(b_m) \\
 & = \frac{N + N2\epsilon}{N + 2\epsilon} + 2\Gamma_2 \sum_{b_m \in B_t(T_O)} w(b_m) + \\
 & \quad (\Gamma_1 + \Gamma_3) \sum_{b_m \in B_f(T_O)} w(b_m) \\
 & = \phi_{FKM}(C', T_O) .
 \end{aligned}$$

□

**Lemma 26.** *If  $O$  is locally optimal for  $(C', \omega, N)$ , then  $O$  is reasonable*

*Proof.* Still, each  $b_m^i \in C'$  has four adjacent points. Assume to the contrary that there is an  $n \in [N]$ , such that  $x_n, \bar{x}_n \notin O$ .

*Case 1:*  $b_m^i \in O$ ,  $b_m^i = \{x_o, x_p\}$ . Similar to before, we observe that exchanging  $b_m^i$  for some other mean can only increase the cost of its adjacent points. All other points have  $b_m^i$  as a mean at distance  $1 + 2\epsilon$ , thus an exchange can not move the mean farther away, hence their cost can not increase.

*Case 1.1:*  $x_o, \bar{x}_o, x_p, \bar{x}_p \notin O$ . Let  $r$  be the optimal memberships of  $C'$  with respect to  $O$ ,  $\tilde{r}$  be the optimal memberships with respect to  $\tilde{O} = (O \setminus \{b_m^i\}) \cup \{x_o\}$ , denote

$$O(x) = \sum_{o \in O \setminus \{b_m^i\}} r(x, o)^2 \|x - o\|^2 \quad \text{and} \quad \tilde{O}(x) = \sum_{o \in O \setminus \{b_m^i\}} \tilde{r}(x, o)^2 \|x - o\|^2 .$$

$$\begin{aligned}
 & \phi_{FKM}(C', O) - \phi_{FKM}(C', \tilde{O}) \\
 & \geq \phi_{FKM}(\{b_m^i, x_o, \bar{x}_o, x_p, \bar{x}_p\}, O) - \phi_{FKM}(\{b_m^i, x_o, \bar{x}_o, x_p, \bar{x}_p\}, \tilde{O}) \\
 & = \sum_{x \in \{x_o, \bar{x}_o, x_p, \bar{x}_p\}} \omega(x) (r(x, b_m^i)^2 \|x - b_m^i\|^2 + O(x)) - \\
 & \quad \sum_{x \in \{b_m^i, \bar{x}_o, x_p, \bar{x}_p\}} \omega(x) (\tilde{r}(x, x_o)^2 \|x - x_o\|^2 + \tilde{O}(x))
 \end{aligned}$$

Recall, that we can only increase the cost by substituting for non-optimal memberships.

$$\begin{aligned}
 & \geq \sum_{x \in \{x_o, \bar{x}_o, x_p, \bar{x}_p\}} \omega(x) (r(x, b_m^i)^2 \|x - b_m^i\|^2 + O(x)) - \\
 & \quad \sum_{x \in \{b_m^i, \bar{x}_o, x_p, \bar{x}_p\}} \omega(x) (r(x, b_m^i)^2 \|x - x_o\|^2 + O(x)) \\
 & = \omega(x_o) (r(x_o, b_m^i)^2 \|x_o - b_m^i\|^2 + O(x_o)) - \\
 & \quad \omega(b_m^i) \underbrace{r(b_m^i, b_m^i)^2}_{=1} (\|b_m^i - x_o\|^2 + \underbrace{O(b_m^i)}_{=0}) + \\
 & \quad \sum_{x \in \{\bar{x}_o, x_p, \bar{x}_p\}} \omega(x) r(x, b_m^i)^2 (\|x - b_m^i\|^2 - \|x - x_o\|^2) \\
 & \geq (r(x_o, b_m^i)^2 W - \omega(b_m^i)) \|x_o - b_m^i\|^2 + W r(\bar{x}_o, b_m^i)^2 c\epsilon + \\
 & \quad W(\epsilon - 2\epsilon)(r(x_p, b_m^i)^2 + r(\bar{x}_p, b_m^i)^2)
 \end{aligned}$$

Using Lemma 23 we obtain

$$\geq \left( \frac{1}{4N^2} W - \omega(b_m^i) \right) \|x_o - b_m^i\|^2 - 2W\epsilon =$$

$$(Mw_{max}^B - \omega(b_m^i)) \|x_o - b_m^i\|^2 - 2W\epsilon \geq (M-1)w_{max}^B(1+\epsilon) - 2W\epsilon.$$

Since  $0 < \epsilon \leq \frac{M-1}{9N^2M}$  we finally obtain

$$\geq (M-1)w_{max}^B - 8N^2Mw_{max}^B \frac{M-1}{9N^2M} > 0.$$

*Case 1.2:*  $\bar{x}_p \in O$  and  $x_o, \bar{x}_o \notin O$ .

$$\begin{aligned} & \phi_{FKM}(C', O) - \phi_{FKM}(C', \tilde{O}) \\ & \geq \phi_{FKM}(\{b_m^i, x_o, \bar{x}_o, x_p, \bar{x}_p\}, O) - \phi_{FKM}(\{b_m^i, x_o, \bar{x}_o, x_p, \bar{x}_p\}, \tilde{O}) \\ & \geq \sum_{x \in \{x_o, \bar{x}_o, x_p\}} \omega(x)(r(x, b_m^i)^2 \|x - b_m^i\|^2 + O(x)) - \\ & \quad \sum_{x \in \{b_m^i, \bar{x}_o, x_p\}} \omega(x)(r(x, b_m^i)^2 \|x - x_o\|^2 + O(x)) \\ & = W(r(x_o, b_m^i)^2 \|x_o - b_m^i\|^2 + O(x_o)) - \\ & \quad \omega(b_m^i) \underbrace{r(b_m^i, b_m^i)^2}_{=1} (\|b_m^i - x_o\|^2 + \underbrace{O(b_m^i)}_{=0}) + \\ & \quad \sum_{x \in \{\bar{x}_o, x_p\}} \omega(x)r(x, b_m^i)^2 (\|x - b_m^i\|^2 - \|x - x_o\|^2) \\ & \geq \left(\frac{1}{4N^2}W - \omega(b_m^i)\right) \|x_o - b_m^i\|^2 + Wr(\bar{x}_o, b_m^i)^2\epsilon + Wr(x_p, b_m^i)^2(\epsilon - 2\epsilon) \\ & \geq (Mw_{max}^B - \omega(b_m^i)) \|x_o - b_m^i\|^2 - \epsilon W \\ & \geq (M-1)w_{max}^B \|x_o - b_m^i\|^2 - \epsilon W \geq (M-1)w_{max}^B(1+\epsilon) - \epsilon W \end{aligned}$$

Since  $0 < \epsilon \leq \frac{M-1}{9N^2M}$  we finally obtain

$$\geq (M-1)w_{max}^B - 4N^2Mw_{max}^B \frac{M-1}{9N^2M} > 0.$$

*Case 1.3:*  $\bar{x}_p \in O, \bar{x}_o \in O$ .

$$\begin{aligned} & \phi_{FKM}(C', O) - \phi_{FKM}(C', (C \setminus \{b_m^i\}) \cup \{x_n\}) \\ & \geq \phi_{FKM}(\{b_m^i, x_o, \bar{x}_o, x_p, \bar{x}_p, x_n, \bar{x}_n\}, O) - \\ & \quad \phi_{FKM}(\{b_m^i, x_o, \bar{x}_o, x_p, \bar{x}_p, x_n, \bar{x}_n\}, (C \setminus \{b_m^i\}) \cup \{x_n\}) \\ & \geq \sum_{x \in \{x_o, x_p, x_n, \bar{x}_n\}} \omega(x)(r(x, b_m^i)^2 \|x - b_m^i\|^2 + O(x)) - \\ & \quad \sum_{x \in \{b_m^i, x_o, x_p, \bar{x}_n\}} \omega(x)(r(x, b_m^i)^2 \|x - x_n\|^2 + O(x)) \\ & = W(r(x_n, b_m^i)^2 \|x_n - b_m^i\|^2 + O(x_n)) - \\ & \quad \omega(b_m^i) \underbrace{r(b_m^i, b_m^i)^2}_{=1} (\|b_m^i - x_n\|^2 + \underbrace{O(b_m^i)}_{=0}) + \\ & \quad \sum_{x \in \{x_o, x_p, \bar{x}_n\}} \omega(x)r(x, b_m^i)^2 (\|x - b_m^i\|^2 - \|x - x_n\|^2) \\ & \geq \left(\frac{1}{4N^2}W - \omega(b_m^i)\right)(1+2\epsilon) + Wr(\bar{x}_n, b_m^i)^2 2\epsilon + \\ & \quad W(r(x_o, b_m^i)^2 + r(x_p, b_m^i)^2)(\epsilon - 2\epsilon) \\ & \geq (Mw_{max}^B - \omega(b_m^i))(1+2\epsilon) - 2\epsilon W \geq (M-1)w_{max}^B(1+2\epsilon) - 2\epsilon W \end{aligned}$$

Since  $0 < \epsilon \leq \frac{M-1}{9N^2M}$  we finally obtain

$$\geq (M-1)w_{max}^B - 8N^2Mw_{max}^B \frac{M-1}{9N^2M} > 0.$$

*Case 2:* There is no  $m \in [M], i \in [3] : b_m^i \in O$ , hence  $\exists o, o \neq n : x_o, \bar{x}_o \in O$ .  $B(x_o) = \{b_m^i \in B \mid x_o \in b_m^i \vee \bar{x}_o \in b_m^i\}$ ,  $|B(x_o)| < M$  (otherwise just exchange  $x_o$  for  $\bar{x}_o$  in the following argument). Observe that

$$\begin{aligned} \phi_{FKM}(B(x_o) \cup \{x_o, x_n, \bar{x}_n\}, O) &= \underbrace{\frac{W(2+4\epsilon)}{N}}_{\phi_{FKM}(\{x_n, \bar{x}_n\}, O)} + \\ &\quad \sum_{b_m^i \in B(x_o)} \omega(b_m^i) \sum_{c \in C} r(b_m^i, c)^2 \|b_m^i - c\|^2. \end{aligned}$$

The only points whose cost can increase by removing  $x_o$  from  $C$  are the points in  $B(x_o)$  and  $x_o$  itself. All points in  $C \setminus (B(x_o) \cup \{x_o\})$  are at distance  $1 + 2\epsilon$  anyways, and hence exchanging  $x_o$  for some other mean can not increase their cost. We obtain

$$\begin{aligned} &\phi_{FKM}(B(x_o) \cup \{x_o, x_n, \bar{x}_n\}, (C \setminus \{x_o\}) \cup \{x_n\}) \\ &\leq \underbrace{\frac{W(2+4\epsilon)}{N+2\epsilon}}_{\phi_{FKM}(\{x_o, \bar{x}_n\}, (C \setminus \{x_o\}) \cup \{x_n\})} + \\ &\quad \sum_{b_m^i \in B(x_o)} \omega(b_m^i) \left( r(b_m^i, x_o)^2 \underbrace{\|b_m^i - x_n\|^2}_{=1+2\epsilon \leq 1+2\epsilon} + \sum_{c \in C \setminus \{x_o\}} r(b_m^i, c)^2 \|b_m^i - c\|^2 \right) \\ &\leq \frac{W(2+4\epsilon)}{N+2\epsilon} + \\ &\quad \sum_{b_m^i \in B(x_o)} \omega(b_m^i) \left( r(b_m^i, x_o)^2 (\|b_m^i - x_o\|^2 + \epsilon) + \sum_{c \in C \setminus \{x_o\}} r(b_m^i, c)^2 \|b_m^i - c\|^2 \right) \\ &= \frac{W(2+4\epsilon)}{N+2\epsilon} + \epsilon \sum_{b_m^i \in B(x_o)} \omega(b_m^i) r(b_m^i, x_o)^2 + \\ &\quad \sum_{b_m^i \in B(x_o)} \omega(b_m^i) \sum_{c \in C} r(b_m^i, c)^2 \|b_m^i - c\|^2 \\ &< \frac{W(2+4\epsilon)}{N+2\epsilon} + \epsilon Mw_{max}^B + \sum_{b_m^i \in B(x_o)} \omega(b_m^i) \sum_{c \in C} r(b_m^i, c)^2 \|b_m^i - c\|^2 \\ &= \frac{W(2+4\epsilon)}{N+2\epsilon} + \epsilon \frac{W}{4N^2} + \sum_{b_m^i \in B(x_o)} \omega(b_m^i) \sum_{c \in C} r(b_m^i, c)^2 \|b_m^i - c\|^2 \\ &< \frac{W(2+4\epsilon)}{N+2\epsilon} + \frac{\epsilon W}{N+2\epsilon} + \sum_{b_m^i \in B(x_o)} \omega(b_m^i) \sum_{c \in C} r(b_m^i, c)^2 \|b_m^i - c\|^2 \\ &< \frac{W(2+4\epsilon) + \frac{2\epsilon(2+4\epsilon)W}{N}}{N+2\epsilon} + \sum_{b_m^i \in B(x_o)} \omega(b_m^i) \sum_{c \in C} r(b_m^i, c)^2 \|b_m^i - c\|^2 \\ &= \frac{W(2+4\epsilon)(1 + \frac{2\epsilon}{N})}{N(1 + \frac{2\epsilon}{N})} + \sum_{b_m^i \in B(x_o)} \omega(b_m^i) \sum_{c \in C} r(b_m^i, c)^2 \|b_m^i - c\|^2 \\ &= \frac{W(2+4\epsilon)}{N} + \sum_{b_m^i \in B(x_o)} \omega(b_m^i) \sum_{c \in C} r(b_m^i, c)^2 \|b_m^i - c\|^2 \\ &= \phi_{FKM}(B(x_o) \cup \{x_o, x_n, \bar{x}_n\}, O) \end{aligned}$$

□

**Corollary 27.** *If  $O$  is locally optimal for  $(C', \omega, N)$ , then  $T_O$  is locally optimal for  $(B, w)$ .*

Proving tightness of  $(\Phi, \Psi)$  and embedding of  $C'$  into  $\ell_2^2$  follows the same line of arguments presented for DISCRETE  $K$ -MEANS in Section 4.

## 6 Open Problems

In this work, we explore the local search complexity of the single-swap heuristic for MUFL and DKM. While we prove that the problem is tightly PLS-complete in general, our reduction requires arbitrarily many dimensions, number of clusters and a non trivial weight function on the clients. One of the first follow-up question is if we can reduce the number of dimensions  $D$  down to a constant. Moreover, it is interesting to examine whether we can obtain our results for unweighted variants of these problems. The fact that the  $K$ -means method has exponential worst-case runtime even for unweighted point sets with  $D = 2$  indicates that this might be possible. A potential approach to reduce the number of dimension is e.g. to embed our abstract point set using different techniques than the one presented here, since this is the only point in the proof that requires high dimensionality.

The major open result is still the conjecture of Roughgarden and Wang, that computing a local minimum of the  $K$ -means algorithm is a PLS-hard problem [RW16].

## References

- [AGK<sup>+</sup>04] V. Arya, N. Garg, R. Khandekar, A. Meyerson, K. Munagala, and V. Pandit. Local Search Heuristics for k-Median and Facility Location Problems. *SIAM Journal on Computing*, 33(3):544–562, 2004.
- [APR14] I. Adler, C. Papadimitriou, and A. Rubinfeld. *On Simplex Pivoting Rules and Complexity Theory*, pages 13–24. Springer International Publishing, 2014.
- [CAKM16] V. Cohen-Addad, P. N. Klein, and C. Mathieu. Local Search Yields Approximation Schemes for k-Means and k-Median in Euclidean and Minor-Free Metrics. *2016 IEEE 57th Annual Symposium on Foundations of Computer Science (FOCS)*, 2016.
- [Dun73] J. C. Dunn. A Fuzzy Relative of the ISODATA Process and Its Use in Detecting Compact Well-Separated Clusters. *Journal of Cybernetics*, 3(3), 1973.
- [FRR16] Z. Friggstad, M. Rezapour, and Salavatipour M. R. Local Search Yields a PTAS for k-Means in Doubling Metrics. *2016 IEEE 57th Annual Symposium on Foundations of Computer Science (FOCS)*, 2016.
- [FS15] J. Fearnley and R. Savani. The Complexity of the Simplex Method. In *Proceedings of the Forty-Seventh Annual ACM on Symposium on Theory of Computing*, STOC '15, pages 201–208, 2015.
- [GK99] S. Guha and S. Khuller. Greedy Strikes Back: Improved Facility Location Algorithms. *Journal of Algorithms*, 31(1), 1999.
- [JHY88] D. S. Johnson, Papadimitriou C. H., and M. Yannakakis. How easy is local search? *Journal of Computer and System Sciences*, 37(1), 1988.
- [JMS02] K. Jain, M. Mahdian, and A. Saberi. A New Greedy Approach for Facility Location Problems. In *Proceedings of the Thirty-fourth Annual ACM Symposium on Theory of Computing*, STOC '02, pages 731–740, 2002.
- [JV01] K. Jain and V. V. Vazirani. Approximation Algorithms for Metric Facility Location and k-Median Problems Using the Primal-dual Schema and Lagrangian Relaxation. *J. ACM*, 48(2):274–296, 2001.



- [KMN<sup>+</sup>04] T. Kanungo, D. M. Mount, N.S. Netanyahu, C. D. Piatko, R. Silverman, and A. Y. Wu. A Local Search Approximation Algorithm for k-Means Clustering. *Computational Geometry*, 28(2), 2004.
- [Llo82] S. Lloyd. Least squares quantization in pcm. *IEEE Transactions on Information Theory*, 28(2), 1982.
- [MDT10] B. Monien, D. Dumrauf, and T. Tscheuschner. *Local Search: Simple, Successful, But Sometimes Sluggish*. Springer Berlin Heidelberg, 2010.
- [PSY90] C. H. Papadimitriou, A. A. Schäffer, and M. Yannakakis. On the Complexity of Local Search. In *Proceedings of the Twenty-second Annual ACM Symposium on Theory of Computing*, STOC '90, 1990.
- [RW16] T. Roughgarden and J.R. Wang. The Complexity of the  $k$ -means Method. In *24th European Symposium on Algorithms*, ESA '16, 2016.
- [Sch38] J. Schoenberg. Metric spaces and positive definite functions. *Transactions of the American Mathematical Society*, 1938.
- [STA97] D. B. Shmoys, É. Tardos, and K. Aardal. Approximation Algorithms for Facility Location Problems. In *Proceedings of the Twenty-ninth Annual ACM Symposium on Theory of Computing*, STOC '97, pages 265–274, 1997.
- [SY91] A. A. Schäffer and M. Yannakakis. Simple Local Search Problems that are Hard to Solve. *SIAM Journal on Computing*, 20(1), 1991.
- [Tor52] W. S. Torgerson. Multidimensional Scaling: I. Theory and Method. *Psychometrika*, 17(4), 1952.
- [Vat11] A. Vattani. k-means Requires Exponentially Many Iterations Even in the Plane. *Discrete & Computational Geometry*, 45(4):596–616, 2011.